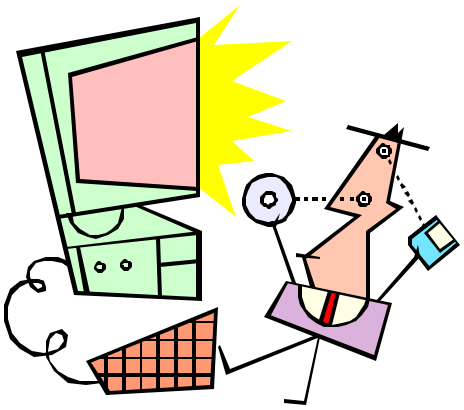

Chemistry 210 Independent Projects Spring 2002

Part of the demonstration that you have reached a level of proficiency in using the computer as a tool to do chemistry and present chemistry is the completion and presentation of an independent project. This project will reflect your interests and will not require you to go beyond your particular level in the chemistry curriculum. Your project may be an extension of an assignment completed earlier in the course, a computer application based on your undergraduate research, an activity you have encountered in another course, or something else you might suggest to your instructor. You must decide on a project *before* May 3. These projects must be completed and published on the web *no later than* 5pm on May 25, and all of you must complete a peer review of each other's projects before the end of finals week.

Some possibilities:

1. Gather information from the rest of the class on the electrostatic potentials and the pK_a's of the acids analyzed in the Spartan assignment. Analyze this data for any correlations. Present the analysis in graphical form and write a short discussion/explanation.
2. Gather similar information about the nitrogen bases, the enthalpy of proton transfer and the pK_b's. Again, analyze the data for any correlations, present the analysis in graphical form and write a short discussion/explanation.
3. Conduct a theoretical study of the internal rotation barriers in a) nitrotoluenes; b) nitrophenols; c) nitroanilines. You would discuss the energy barriers and associated potential energies around the C-NO_2 bond. Dr. K. can provide you with references.
4. Examine the possible role for π-stacking in the self-assembly of amyloid fibrils. Dr. K. can provide you with references.
5. Coduct an analysis of “antigene” strategy. Oligonucleotide triple helix formation is a unique way to design specific ligands that recognize

double-stranded DNA. Oligonuelcotides of defined sequence can bind to the major groove of DNA to form triple helices. Dr. K. can provide you with references.

6. Use Spartan to graphically represent an chemical reaction of your choice. For example, you might consider the pinacol and benzpinacol rearrangement: is a bridged intermediate favorable?
7. Imagine you are studying an enzyme mechanism that is believed to involve a proton transfer step which utilizes the imidizole ring of a histidine residue. Predict the preferred site for protonation of 4-methyl imidazole. Explain your reasoning.
8. Analyze the structure changes that occur in prion proteins. Dr. K. can provide you with some references.
9. Analyze the structure changes that occur in proteins when 40 glutamine residues are inserted…this is the basis for a number of diseases. Dr. K. can provide you with some references.
10. Use the vibrational frequency data for acetic acid to construct its infrared spectrum. For this, you will need to calculate the intensities of the vibrational bands. Use Mathematica or Excel to plot it.
11. All calculations we have done with Spartan have been done in vacuo. You might want to look at the effect of solvent on potentials, equilibrium constants, etc…
12. Analyze the kinetics of a reaction.
13. Examine interactions of drugs with DNA.
14. Examine the effect of nucleotide bulges on the stability and topology of RNA.
15. Examine the effect of nucleotide sequence on the structure of DNA.
16. Model polystyrene, and compare this to models that include various percentages (1, 2, 4, 8, 10%) replacement of the phenyl groups by tri-*n*-butyltin chloride and hydride.